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A Piecewise Linear Finite Element Discretization of the Diffusion Equation for Arbitrary Polyhedral Grids

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ABSTRACT

We develop a piecewise linear (PWL) Galerkin finite element spatial discretization for the multidimensional radiation diffusion equation. It uses recently introduced piecewise linear weight and basis functions in the finite element approximation and it can be applied on arbitrary polygonal (2D) or polyhedral (3D) grids. We first demonstrate some analytical properties of the PWL method and perform a simple mode analysis to compare the PWL method with Palmer's finitevolume method and with a bilinear continuous finite—element method. We then show that this new PWL method gives solutions comparable to those from Palmer's. However, since the PWL method produces a symmetric positive definite coefficient matrix, it should be substantially more computationally efficient than Palm er's method, which produces an asymm etric matrix. We conclude that the Galerkin PWL method is an attractive option for solving diffusion equations on unstructured grids.

KEYWORDS: diffusion, arbitrary polyhedral grids, piecewise linear finite element

1. INTRODUCTION

Several methods have been developed to solv e the radiation diffusion equation on arbitrar y polyhedral (3D) and polygonal (2D) meshes. A finite-volume (FV) method developed by Palmer [1,2] divides each cell into "corner" subcells and enforces conservation on each dual cell, where a dual cell is the union of corners that touch a vertex. This method is second-order accurate, with relatively small error norms, and is exact on any grid if the exact solution is linear in the position variables. However, Palmer's method does not generate a symmetr ic coefficient matrix, so the matrix system is (rela tively) computationally expensive to store and solve. W achspress previously developed rational-polynomial basis functions [3] that can be applied to polyhedral cells in a finite-element method (FEM). His functions have the advantage that a Galerkin FEM formulation will yield a symmetric positive definite (SPD) matrix, but the disadvantage that the basis-function integrals must be done numerically.

In this work we apply a rela tively new FEM basis function – the "Piece Wise Linear" (PWL) function [4] – to the radiation diffusion equation on arbitrary polygonal and polyhedral meshes. The goals are to gain an SPD coefficient matrix, retain the simplicity and accuracy of Palmer's

finite-volume method, and avoid the num erical integrations that plague W achspress's method. As part of our development we show that in most cases Palmer's method is, in fact, a FEM with PWL basis functions, but with Pe trov-Galerkin weighting. (The weight functions are constants over dual cells.) We then show that the PWL method produces a well-posed discrete problem, and we show that the PWL method will have sec ond-order convergence properties. To further characterize the methods we performed a simple mode analysis on the lum ped and unlum ped PWL methods, Palm er's method, and the lumped and unlum ped bilinear continuous finite element methods (BLC). We compare our Galerkin PWL method against Palm er's method on multiple test problems. We find that our method meets all of our goals: it yields accuracy comparable to Palm er's method, produces an SPD matrix, and involves only very simple integrations.

We remark that this is an active field of res earch, with methods constantly under development. For example, Morel has proposed a cell-centered FV m ethod for polyhedral cells [5], and support-operator methods have been proposed by Kuznetsov et al. [6]. We do not claim that our PWL FEM is superior to these m ethods for all problems. Further research is needed to determine which methods are best for different applications.

2. DEVELOPMENT

2.1 Introduction

An asymptotic limit of the ra diation transport equation is a time-dependent radiation conservation equation [7]:

$$a\frac{\partial}{\partial t} \left(T^{(0)}(\vec{r},t)\right)^4 - \vec{\nabla} \cdot \frac{ac}{3\sigma_R} \nabla \left(T^{(0)}(\vec{r},t)\right)^4 = Q(\vec{r},t), \tag{1}$$

For simplicity we express Eq. (1) as

$$\frac{1}{c}\frac{\partial}{\partial t}E(\vec{r},t) - \vec{\nabla} \cdot D\vec{\nabla}E(\vec{r},t) = Q(\vec{r},t)$$
(2)

where E is the rad iation energy density, Q is the source, and D is a diffusion coefficient. We begin discretizing Eq. (2) by applying a simple fully-implicit Euler approximation to the time derivative, which results in

$$\frac{1}{c} \frac{\left(E^{n+1}(\vec{r}) - E^n(\vec{r})\right)}{\Delta t} - \vec{\nabla} \cdot D\vec{\nabla} E^{n+1}(\vec{r}) = Q^n(\vec{r}), \tag{3}$$

where the *n* superscripts represent the time-step index. In Eq.(3), we solve for E^{n+1} to obtain a diffusion equation.

$$-\vec{\nabla} \cdot D\vec{\nabla} E^{n+1}(\vec{r}) + \sigma E^{n+1}(\vec{r}) = S^n(\vec{r}), \tag{4}$$

where

$$\sigma = \frac{1}{c\Delta t} \tag{5}$$

and

$$S^{n}(\vec{r}) = Q^{n}(\vec{r}) + \frac{1}{c\Delta t}E^{n}(\vec{r}). \tag{6}$$

Eq. (4) is the final form of the steady state diffusion equation to which we will apply all spatial discretizations. We also define the net current vector:

$$\vec{F} = -D\vec{\nabla}E \ . \tag{7}$$

2.2 Galerkin PWL FEM

To apply an FEM to the diffusion equation, we first multiply the equation by a weight function and integrate it over the problem domain. If the *i*-th weight function is nonzero only on cells that touch the *i*-th vertex, then we have

$$\int_{z \, ati} d^3 r \, w_i(r) \left[-\vec{\nabla} \cdot D \vec{\nabla} E(\vec{r}) + \sigma E(\vec{r}) - S(\vec{r}) \right] = 0 \,, \tag{8}$$

where z denotes cells (which we sometimes call "zones"). The divergence theorem produces:

$$\int_{\partial z \, at \, i} d^2 r \, w_i(\vec{r}) \vec{n} \cdot \vec{F} + \int_{z \, at \, i} d^3 r \left[D \vec{\nabla} E(\vec{r}) \cdot \vec{\nabla} w_i(\vec{r}) + w_i(\vec{r}) (\sigma E(\vec{r}) - S(\vec{r})) \right] = 0.$$
 (9)

The first term is zero if the cells over which the equation is integrated are not on the boundary of the domain. We ignore it in the remainder of this development. An approximation can be made for *E* in terms of known basis functions:

$$E(\vec{r}) = \sum_{all \ j} E_j b_j(\vec{r}), \tag{10}$$

which results in

$$\sum_{j} E_{j} \left\{ \int_{z \, ati} d^{3}r \left[D \vec{\nabla} b_{j}(\vec{r}) \cdot \vec{\nabla} w_{i}(\vec{r}) + \sigma b_{j}(\vec{r}) w_{i}(\vec{r}) \right] \right\} = \int_{z \, ati} d^{3}r \, w_{i}(\vec{r}) S(\vec{r}). \tag{11}$$

Eq. (11) is N equations for N unknowns. Given our assumption of one weight function per vertex, N is the number of vertices in the mesh.

A Galerkin FEM sets $w_i = b_i$. It is not difficult to show that this yields a symmetric positive-definite matrix. In this work we develop a Galerk in FEM that em ploys the piece wise linear (PWL) weight and basis function s developed recently by Stone and Adams [4]. In the development of vertex-centered m ethods for arbitrary polyhedral cells, each polyhedral cell is divided into subcell volum es called sides, corners, and wedges. A side is a tetrahedron made from two adjacent vertices, the zone center, and a face center. A corner, which will be used

primarily in the developm ent of Palmer's finite volume method, is defined as the union of all half-sides that touch a vertex in one zone. A wedge is defined to be a half side. See Figures 1, 2, and 3 for depictions of side subcells, corner subcells, and wedges in a hexahedral cell.

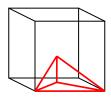


Figure 1: Side in a hexahedral cell

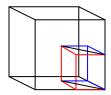


Figure 2: Corner in a hexahedral cell

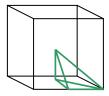


Figure 3: Wedge in a hexahedral cell

The PWL function centered at vertex *j* can be written in three dimensions as:

$$b_{j}(\vec{r}) = t_{j}(\vec{r}) + \sum_{\text{faces at } j} \beta_{f,j} t_{f}(\vec{r}) + \alpha_{z,j} t_{z}(\vec{r}),$$
 (12)

where the t functions are standard linear functions—defined tetrahedron by tetrahedron. For example, t_j equals 1 at the j-th vertex and decreases linearly to zero on all other vertices of each side that touches point j. t_z is unity at the cell midpoint and zero at each face midpoint and each cell vertex. t_f is unity at the face midpoint and zero at the cell midpoint and at each of the face's vertices. The α_z and β_f are weights that give the cell and face midpoints as weighted averages of their vertices:

$$\vec{r}_z = \text{cell midpoint} = \sum_{j@z} \alpha_{z,j} \vec{r}_j;$$
 (13)

$$\vec{r}_f \equiv \text{cell midpoint} = \sum_{j@f} \beta_{f,j} \vec{r}_j$$
 (14)

Each basis function is piecewis e linear on each side, which m akes integration over sides straightforward. (Note that the gradient of a basis function is constant on a side.) Figure 4 shows a plot of a PWL basis function for a two-dimensional rectangular cell.

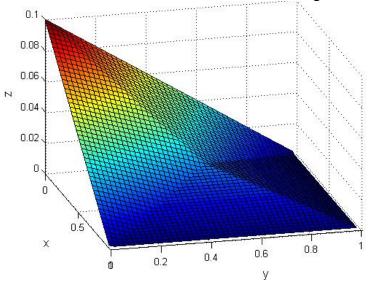


Figure 4: 2D Piecewise Linear Basis Functions

The definitions in Eqs. (12)-(14) guarantee that any linear function of (x,y,z) can be exactly represented as an expansion in these basis functions. (This sub tlety is what makes the method work. Effectively, the functions generate interpolated values at cell and face midpoints, in such a way that the interpolated values are perfect for linear functions.)

Our Galerkin FEM uses PWL functions for the w and b in the general equation above, with one exception: we *lump* the "mass matrix." That is, we make the replacement:

$$\int_{z@i} d^3r \left[\sigma b_j(r) w_i(r) \right] \xrightarrow{lump} \delta_{ij} \int_{c@i} d^3r \left[\sigma \right], \tag{15}$$

where c refers to a "corner" subcel 1. On orthogonal grids with σ constant in each cell, this is equivalent to standard FEM m ass-matrix lumping, because the volume of the corner at each vertex and the integral of the weight function over the cell both equal 1/8 of the cell volume (or 1/4 of the cell area in 2D). On general g rids, however, Eq. (15) is not equivalent to standard mass-matrix lumping. We choose this non-s tandard lumping so that our source and collis ion terms are identical to those in Palmer's method, thus allowing our study to focus on different treatments of the diffusion term.

This completes the definition of our new m ethod (except for boundary conditions, which are straightforward).

2.3 Palmer's Finite-Volume Method

Palmer's method is developed by dividing each cell into corners, defining dual cells to be the union of corners at each vertex, and enforcing conservation over these dual cells. The gradient

of the scalar flux is taken to be constant within each wedge subcell, and the cell-center scalar flux is an interpolant of the vertex scalar fluxes, defined such that it is exact for functions that are linear in x, y, and z. The method enforces continuity of particle flow (the normal component of the current) across each dual cell boundary. See references [1] and [2] for more details.

It is interesting to note that in most cases Palmer's FV method is equivalent to a Petrov-Galerkin FEM with PW L basis functions, with the mass-matrix lumping defined above, and with a constant diffusion coefficient in each side subcell volume. The weight functions for this case are given by:

$$w_i(\vec{r}) = \begin{cases} 1, & \vec{r} \in \text{ any corner that touches vertex } i, \\ 0, & \text{otherwise.} \end{cases}$$
 (16)

As far as we know, this has not been previously observed. This illuminates the close connection between Palmer's method and our Galerkin FEM, and it also may permit Palmer's method to be better understood and analyzed. The exceptions to this interpretation occur when the diffusion coefficient, D, is allowed to vary within a cell. In such cases, Palm er's method does not assume that E varies linearly within each side, but instead allows E's slope to change so that $\vec{n} \cdot D\vec{\nabla}E$ is the same in both wedges where they meet inside one side.

Both methods should be exact (within the lim its of roundoff error) if the solution is a linear function of x, y, and z, regardless of how distorted the spatial cells become. (We test this below.) This follows from the construction of the PWL basis functions.

3. ANALYSES OF PWL AND RELATED METHODS

3.1 Well-Posedness

Using the Lax-Milgram Lemma, we can sho w that the PW L discretization of the diffusion equation results in a well-posed di screte problem. This discrete problem is derived from the weak formulation of the diffusion equation:

$$\int_{\Omega} d\Omega \vec{\nabla} v \cdot \vec{\nabla} u + \lambda \int_{\Omega} d\Omega v u = \int_{\Omega} d\Omega v f,$$

$$u \in H_0^1(\Omega) \text{ and } \forall v \in H_0^1(\Omega),$$
(17)

where $H_0^1(\Omega)$ is a Hilbert space with the norm:

$$\|w\|_{H_0^1(\Omega)} = \left(\|\nabla w\|_{L^2}^2 + \|w\|_{L^2}^2\right)^{1/2}.$$
 (18)

Here λ plays the role of σ/D . Also for simplicity, define

$$a(u,v) = \int_{\Omega} d\Omega \vec{\nabla} v \cdot \vec{\nabla} u + \lambda \int_{\Omega} d\Omega v u$$

$$S(v) = \int_{\Omega} d\Omega v f$$
(19)

The Lax-Milgram Lemma [8] states that a problem is well-posed (a solution exists and is unique) if

- 1. The weight and basis (or test and trial) functions are in a Hilbert space, H
- 2. a(u,v) is a bilinear form on H
- 3. a(u,v) is bounded
- 4. a(u,u) is coercive
- 5. S(v) is linear and bounded

The first two elements of the lemma are obviously satisfied. To prove the third element, we start by taking the absolute value of a(u,v) and writing the integrals in terms of norms.

$$|a(u,v)| \le \int_{\Omega} d\Omega |\vec{\nabla} u \cdot \vec{\nabla} v| + |\lambda| \int_{\Omega} d\Omega |uv| \le ||\nabla u||_{L^{2}} ||\nabla v||_{L^{2}} + |\lambda| ||u||_{L^{2}} ||v||_{L^{2}}.$$
 (20)

Applying the Cauchy-Schwarz inequality and performing some algebra yields:

$$|a(u,v)| \le (1+\lambda) \left(\|\nabla u\|_{L^{2}}^{2} + \|u\|_{L^{2}}^{2} \right)^{1/2} \left(\|\nabla v\|_{L^{2}}^{2} + \|v\|_{L^{2}}^{2} \right)^{1/2} = (1+\lambda) \|u\|_{H^{1}(\Omega)} \|v\|_{H^{1}(\Omega)}. \tag{21}$$

We now see that a(u,v) is bounded because

$$\frac{\left|a\left(u,v\right)\right|}{\left\|u\right\|_{H^{1}(\Omega)}\left\|v\right\|_{H^{1}(\Omega)}} \le \left(1+\lambda\right) < \infty \tag{22}$$

for all non-zero u and v.

The next step is to prove that a is coercive:

$$a(u,u) = \int_{\Omega} d\Omega \vec{\nabla} u \cdot \vec{\nabla} u + \lambda \int_{\Omega} d\Omega (u)^{2} = \|\nabla u\|_{L^{2}}^{2} + \lambda \|u\|_{L^{2}}^{2} \ge \alpha \left\{ \|\nabla u\|_{L^{2}}^{2} + \|u\|_{L^{2}}^{2} \right\}, \tag{23}$$

or

$$a(u,u) \ge \alpha \|u\|_{H^1(\Omega)}^2,\tag{24}$$

where $\alpha = \min(1, \lambda)$. Thus, as long as $\frac{\sigma}{D} > 0$, a is coercive.

The final step is to prove that S(v) is bounded:

$$|S(v)| = \int_{\Omega} d\Omega |v| |f| \le ||f||_{L^{2}} ||v||_{L^{2}} \Rightarrow \sup_{v \ne 0} \left\{ \frac{|S(v)|}{||v||_{L^{2}(\Omega)}} \right\} \le ||f||_{L^{2}(\Omega)} < \infty . \tag{25}$$

Thus, S(v) is bounded if the original source function is bounded in the L $_2$ norm. For our problems of interest this is all ways true. We conclude that the Galerkin PWL method yields a well-posed problem when applied to a diffusion equation with $\sigma/D > 0$.

3.2 Order of Accuracy as Mesh is Refined

By the Bramble-Hilbert Lemma, we know that a discretization utilizing the standard linear basis functions on a tetrahedral m esh will have a second-order convergence rate in the L 2 norm. [8] We can further prove that the PWL method will have a second-order convergence rate if we can prove the difference between the standard interpolation:

$$I_h u = \sum_{j \in h} t_j u(\vec{r}_j) + \sum_{f \in h} t_f u(\vec{r}_f) + t_z u(\vec{r}_z)$$

$$\tag{26}$$

and the PWL interpolation:

$$\tilde{I}_h u = \sum_{j \in h} t_j u(\vec{r}_j) + \sum_{f \in h} t_f \sum_{i \in f} \beta_{f,i} u(\vec{r}_i) + t_z \sum_{j \in h} \alpha_j u(\vec{r}_j)$$
(27)

is also second-order. The difference between Eq. (27) and Eq. (26) is

$$\tilde{I}_h u - I_h u = \sum_{f \in h} t_f^L \left(\sum_{i \in f} \beta_{f,i} u(\vec{r}_i) - u(\vec{r}_f) \right) + t_z^L \left(\sum_{j \in h} \alpha_j u(\vec{r}_j) - u(\vec{r}_z) \right), \tag{28}$$

which will be second-order if

$$\sum_{i \in f} \beta_{f,i} u(\vec{r}_i) - u(\vec{r}_f) = O(h^2)$$
(29)

and

$$\sum_{j \in h} \alpha_j u(\vec{r}_j) - u(\vec{r}_z) = O(h^2). \tag{30}$$

We introduce Taylor series expansions of $u(\vec{r}_i)$ about point \vec{r}_f and of $u(\vec{r}_j)$ about point \vec{r}_z :

$$\sum_{i \in f} \beta_{f,i} u(\vec{r}_i) - u(\vec{r}_f) = \left(\sum_{i \in f} \beta_{f,i} - 1\right) u(\vec{r}_f) + \left(\sum_{i \in f} \beta_{f,i} \left(\vec{r}_i - \vec{r}_f\right)\right) \cdot \nabla u(\vec{r}_f) + O(h^2)$$
(31)

and

$$\sum_{j \in h} \alpha_j u(\vec{r}_j) - u(\vec{r}_z) = \left(\sum_{i \in f} a_j - 1\right) u(\vec{r}_z) + \left(\sum_{i \in f} a_j (\vec{r}_j - \vec{r}_z)\right) \cdot \nabla u(\vec{r}_z) + O(h^2). \tag{32}$$

The summation terms on the right-hand sides vanish if for every face we have:

$$\sum_{i \in f} \beta_{f,i} = 1 \quad \text{and} \quad \sum_{i \in f} \beta_{f,i} \left(\vec{r}_i - \vec{r}_f \right) = 0, \tag{33}$$

and for every cell we have

$$\sum_{j \in h} \alpha_j = 1 \quad \text{and} \quad \sum_{j \in h} \alpha_j \left(\vec{r}_j - \vec{r}_z \right) = 0 . \tag{34}$$

These are in fact the equations that the PW L method uses to determ ine its cell and face midpoints and its basis functions. Thus, we expect the PWL solution to converge like $O(h^2)$ in the L_2 norm.

3.3 Modal Analysis and Comparison of Methods

We have also analyzed a sim ple test problem: infinite medium, 2D, rectangular cells, constant material properties, uniform mesh spacings. From this test problem we can use a sim ple mode analysis to determine how various methods' solutions compare with the analytic solution and with each other.

For this problem, the analytic solution of the diffusion equation can be determined for a source that can be written in terms of Fourier modes. The 2D diffusion equation is:

$$-D\left[\frac{d^2\phi(\vec{r})}{dx^2} + \frac{d^2\phi(\vec{r})}{dy^2}\right] + \sigma_a\phi(\vec{r}) = S(\vec{r}). \tag{35}$$

The source can be expanded as

$$S(\vec{r}) = \int_{-\infty}^{\infty} dw_y \int_{-\infty}^{\infty} dw_x S_{\vec{w}} \exp(i\vec{w} \cdot \vec{r})$$
 (36)

The solution can also be expanded:

$$\phi(\vec{r}) = \int_{-\infty}^{\infty} dw_y \int_{-\infty}^{\infty} dw_x \phi_{\vec{w}} \exp(i\vec{w} \cdot \vec{r}).$$
 (37)

If we substitute Eqs. (36) and (37) into Eq. (35) and perform some algebra, we find that a given mode of the solution is independent of other modes and satisfies:

$$\phi_{\vec{w}} = \frac{S_{\vec{w}}}{D\|w\|^2 + \sigma_a} \,. \tag{38}$$

This analysis can also be applied to solutions of discretized diffusi on equations. We have applied this to five discretization methods: lumped PW L (LPWL), unlumped PWL (UPW L), Palmer's method, lumped bilinear continuous FEM (LBL), and unlumped bilinear continuous FEM (UBL). After extensive but straightforward algebra we find that each method results in a solution of the form:

$$\phi_{\vec{w}} = \frac{S_{\vec{w}}}{D\left\{w_x^2 f_{method}\left(\theta_x, \theta_y\right) + w_y^2 f_{method}\left(\theta_y, \theta_x\right)\right\} + \sigma_a},$$
(39)

where $\theta_x = w_x \Delta x$ and $\theta_y = w_y \Delta y$. Note that if the f factors were unity, the solution would be identical to the analytic solution. Also note that there are two different f factors in Eq. (39): the f function for the given m ethod with the arguments in different orders. The f factors for each method are:

$$f_{LPWL}\left(\theta_x, \theta_y\right) = \left[2\left(\frac{1 - \cos\left(\theta_x\right)}{\theta_x^2}\right)\right] \left[\frac{3 + \cos\left(\theta_y\right)}{4}\right],\tag{40}$$

$$f_{UPWL}(\theta_x, \theta_y) = \left[2\frac{1 - \cos(\theta_x)}{\theta_x^2}\right] \left[\frac{3}{1 + \left[1 + \cos(\theta_x)\right] \frac{5 + 3\cos(\theta_y)}{6 + 2\cos(\theta_y)}}\right], \tag{41}$$

$$f_{Palmer}(\theta_x, \theta_y) = 2\left[\frac{1 - \cos(\theta_x)}{\theta_x^2}\right],$$
 (42)

$$f_{LBL}(\theta_x, \theta_y) = \left[2\left(\frac{1 - \cos(\theta_x)}{\theta_x^2}\right)\right] \left[\left(\frac{2 + \cos(\theta_y)}{3}\right)\right],\tag{43}$$

and

$$f_{UBL}(\theta_x, \theta_y) = \left[2\left(\frac{1 - \cos(\theta_x)}{\theta_x^2}\right)\right] \left[\left(\frac{3}{2 + \cos(\theta_x)}\right)\right]. \tag{44}$$

Each of these factors approaches unity in the fine mesh limit ($\theta_x \to 0$ and $\theta_y \to 0$). We define an error for each method as:

$$\varepsilon_{method} = \left| 1 - f_{method} \right|. \tag{45}$$

The analysis shows that solution accuracy depends not only on the mesh size, which is expected, but also on the "m odes" that are present in the source. If a problem has a non-s mooth source, then high-wavenumber modes (large w values) are required to model the source. For this reason, to obtain accurate numerical results the mesh must resolve the wave numbers required to m odel any non-smooth sources.

Figures 5, 6, 7, 8 and 9 show plots of $\varepsilon_{method}(\theta_x, \theta_y)$ for each method. Because Palmer's and UBL's ε 's depend on only one θ -variable, we have included a plot of both errors in Figure 10.

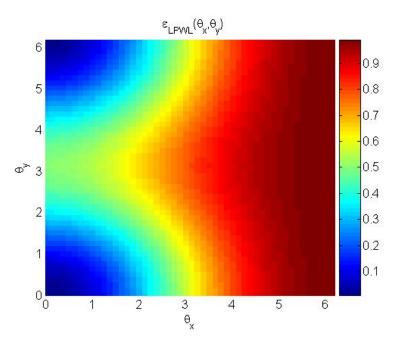


Figure 5: Error for lumped PWL

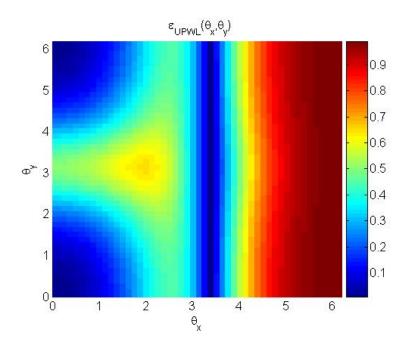


Figure 6: Error for unlumped PWL

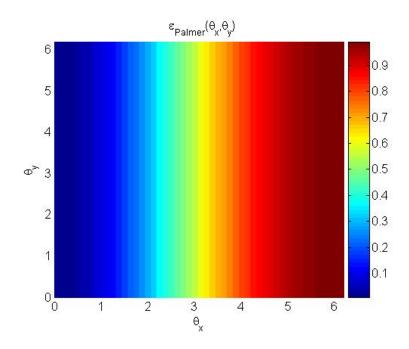


Figure 7: Error for Palmer's method

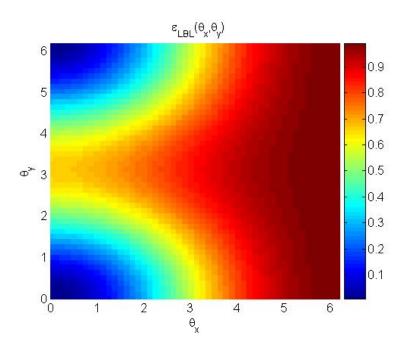


Figure 8: Error for lumped bilinear continuous finite element

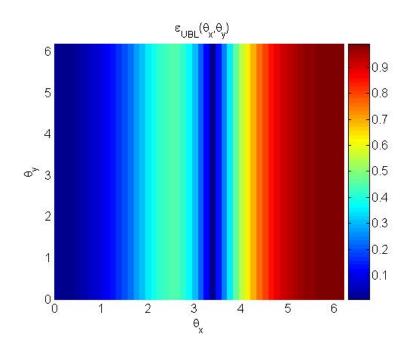


Figure 9: Error for unlumped bilinear continuous finite element

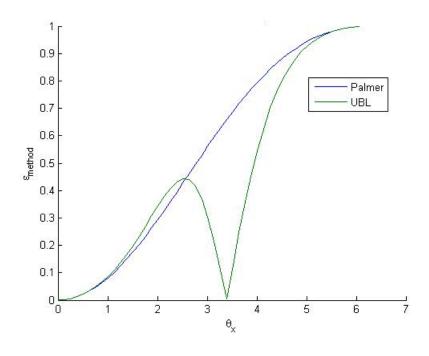


Figure 10: Error comparison of Palmer's method and unlumped bilinear continuous

From these equations and figures it is easy to see that Palm er's method's f factors will always be closer or as close to unity as the f factors of both the lumped PWL and lumped BL methods. In addition, the f values monotonically decrease from a value of unity as the problems move farther from the fine-mesh limit. As a result, for simple homogeneous problems on rectangular grids we

expect Palmer's method to be slightly m ore accurate than the lum ped FEMs for si ngle-mode problems. This result is interesting because we anticipated that Galerkin finite element methods would be more accurate than Petrov-Galerk in finite element methods for discretizing the diffusion operator. When we "unlump" the FEMs, the f factors in the unlumped cases no longer monotonically decrease with increasing cell size. They become larger than unity, and then begin to decrease as the mesh size moves away from the fine-mesh limit. Furthermore, the unlumped FEM f values appear to stay closer to one for a larger range of θ s. From this result, we conclude that we gain some accuracy if we do not lum p (or lose accuracy when we lum p) the FEMs and incur non-monotonic convergence away from the fine-mesh limit. Finally, we notice that the behaviors of the PW L and BL m ethods are strikingly similar, although the accuracy of the lumped PWL method is always better than the accuracy of the lum ped BL method for a given mode, and the accuracy of unlumped BL is always slightly better than the accuracy of unlumped PWL for a given mode. This similarity indicates that the discontinuities in the derivatives of the PWL basis functions do not have a significant impact on the accuracy of the method.

4. RESULTS

4.1 Accuracy

To test our implementation of the Galerkin PW L method as well as the prediction of perfection for linear solutions, we consider a three-dimensional problem with a linear solution that varies only in x. This problem has no source, no absorption, reflecting boundary conditions for the z and y dimensions, and Dirichlét boundary conditions of E(0,y,z)=0 and E(1,y,z)=1. Figures 11 and 12 show contour plots of this solution generated by our Galerkin PWL method on a random mesh and a "Z-mesh."[9] From these plots (and many, similar ones), we conclude that the PWL method does reproduce the exact linear solution. This property is also attained by Palm er's method.

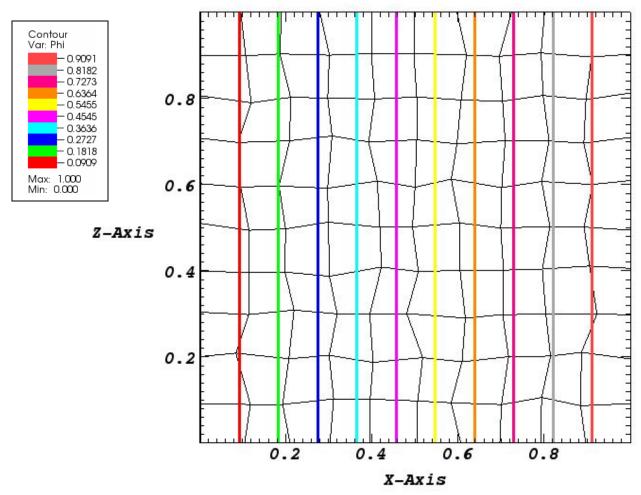


Figure 11: Contour plot of a 1D linear solution on a random mesh at y=0.75. (Solution is the same on other y-planes, as it should be.)

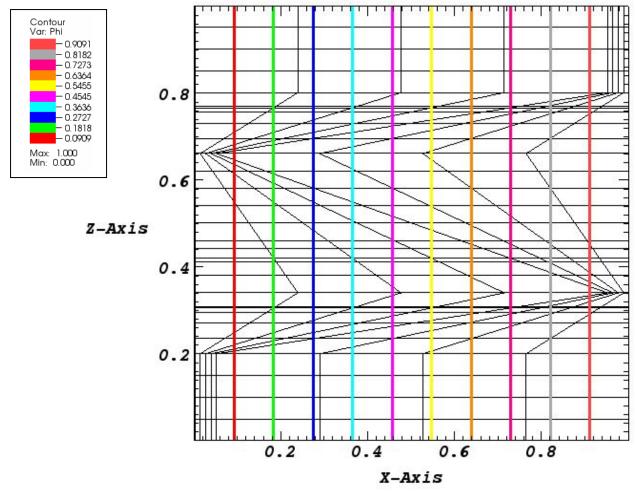


Figure 12: Contour plot of a 1D linear solution on a Z-mesh at *y*=0.75. (Solution is the same on other *y*-planes, as it should be.)

A Z-mesh problem with a linear so lution in x, y, and z was also run to show that the method produces the linear solution on a difficult mesh in all dimensions. This test problem had absorption, a linear source, and applied Dirichlét boundary conditions that enforced a linear solution on each face. Solution contours should be straight diagonal lines, and they are, as we see in Figure 13.

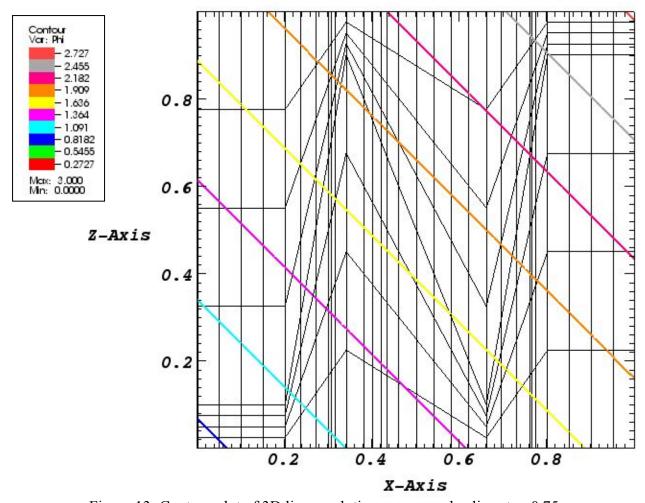


Figure 13: Contour plot of 3D linear solution on a z-mesh, slice at y=0.75

The next set of problem s tests the convergence rate of both the PW L method and Palm er's method on a series of random meshes, and on orthogonal meshes. (Each random mesh was generated by randomly perturbing each non-boundary vertex of an orthogonal mesh.) One test measures the convergence rate for a problem with a known one-dimensional quartic solution. Palmer used this same problem to test the convergence rate of his finite volume method. [1] This problem has no absorption, a quadratic source, and Dirichlét boundary conditions of E(0,y,z)=0 and E(1,y,z)=1. The results from this test are found in Figure 14.

A second test problem was developed to further test the convergence rate. This problem includes absorption, has no source, and Dirichlét boundary conditions of E(0,y,z)=1 and E(1,y,z)=0. It has an exponential solution. The results from this test are also found in Figure 14. The error norm is calculated by taking the L_2 norm of the vector of the exact solution minus the calculated solution. The convergence rate of the methods is determined by the slopes of the lines in Figure 14. If the slope is two on the log-log pl ot, the method has a second-order convergence rate, which means that the error in the solution gets decreased by a factor of four when the m esh is refined by a factor of two. In Figure 14 we plot a reference—line with a slope of exactly two to compare the results of the num erical tests. We also plot—errors from the two test problems described previously. The results from the quartic solution problem appear above the black reference line.

These results show that for this test problem, not much accuracy is lost when the m esh changes from brick to random . The results from the exponential solution problem appear below the reference line. These lines represent the convergence rates of PWL and Palmer's method on random meshes for an exponential solution, and PWL on brick meshes for an exponential solution. These results show that for this test problem, the methods lose about a factor of three in accuracy when the mesh is changed from a brick mesh to a random mesh. In general, both methods show second-order accuracy and have the same magnitude of error for both the quartic problem and the exponential problem

Convergence of the Methods

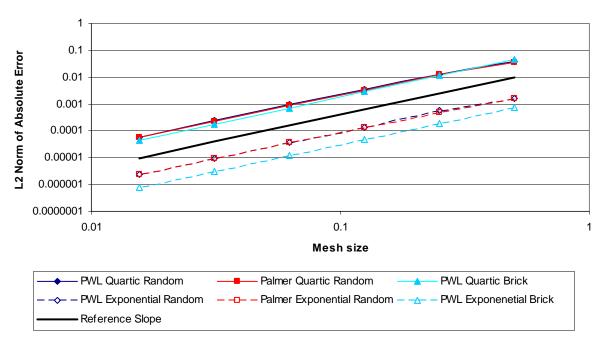


Figure 14: Convergence rates of Palmer's method and PWL on various test problems

We analyzed the Galerkin PWL method in the limit of high aspect ratios on two dimensional orthogonal grids, and found that the signs of the off-diagonal elements in the diffusion matrix will change at certain ratios of Δx and Δy . For $(\Delta x/\Delta y)^2 < 1/3$, the sign change occurs for the vertices that are above and below the central vertex. For $(\Delta y/\Delta x)^2 < 1/3$, the sign change occurs for the vertices to the left and right of the central vertex. Thus, for problems with cells of high aspect ratio, the coefficient matrix is no longer an "M-matrix." This raises the possibility that its inverse could have negative elements, which in turn raises the possibility that in some problems the method could produce unphysical oscillations and/or negative soluitons. To test this we ran a problem on an orthogonal mesh with 64 cells of the 1024 total cells having 1000 to 1 aspect ratios $(\Delta y/\Delta x)$. These cells were contiguous, and inserted into the problem at x=0.375 on a cubical domain of unit width. The test problem had Dirichlét boundary conditions of E(0,y,z)=0, E(1,y,z)=0, E(x,0,z)=0 and E(x,1,z)=0, and reflecting boundary conditions in the z direction. The source in this problem is a "point source" inserted into the problem at only one vertex in the middle of the region containing cells with high aspect ratios. The plot of the PW L solution is

shown for an equally spaced mesh in Figure 15 and a mesh with high aspect ratio cells in Figure 16.

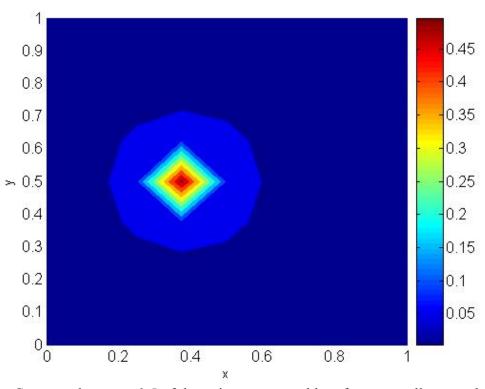
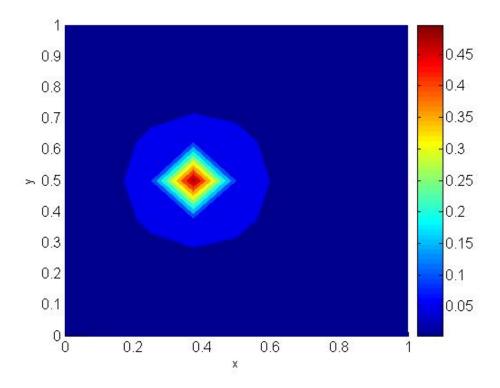


Figure 15: Contour plot at z = 0.5 of the point source problem for an equally spaced mesh with the source at x=0.375 and y=0.5



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Figure 16: Contour plot at z = 0.5 of the point source problem for a mesh with high aspect ratio zones with the source at x=0.375 and y=0.5.

These plots show just a slice of the problem. The slice was taken in the z direction at the value of z where the solution is maximum.

The presence of the high-aspect-ratio cells doe s not affect the solution significantly. In particular, despite the singular source, there are no unphysical oscillations or negative values in the PWL solution, which indicate s that the even though the m atrix is not and "M-m atrix," its inverse has no negative values. The problem s with uniform and non- uniform grids have the same source strength, which is input into bo th problems at a single node with the sam e coordinates. The magnitude of the solution is slightly larger (0.6%) for the problem with the high aspect-ratio cells, but we attribute this small difference to the finer m esh spacing near the source.

4.2 Efficiency

Because PWL produces an SPD m atrix, we can use the Conjugate Gradient (C G) method to solve the matrix system. Palm er's method must be solved using an asymmetric solver such as GMRES. We expect that CG will be more efficient, and we test this conjecture on a tim edependent "tophat" problem, with the radiation diffusion equation coupled to an energy-balance equation for the material (which the material temperature must satisfy). The tophat problem is a two-material problem, with a high-density region and a low-density tophat region. In Figure 17, the red region is the high-density, thick region, and the blue region is the low-density, thin region. While the details are not important for our purposes he re, we note that the material opacities are temperature-dependent and the radiation source is a Planckian at the material temperature.

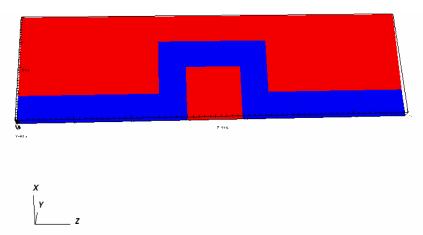
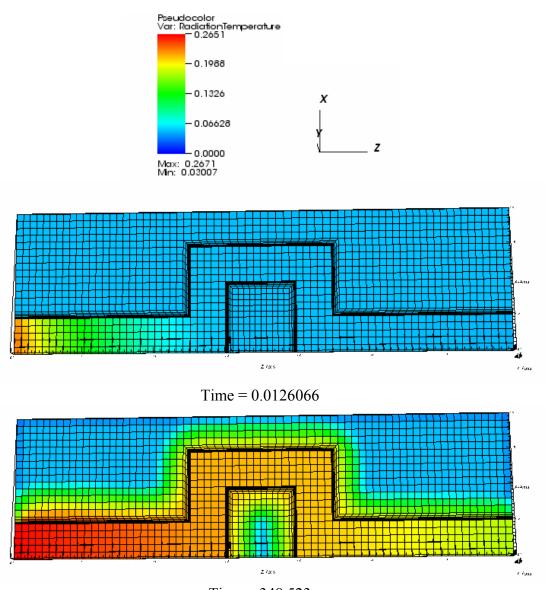


Figure 17: The material densities of the tophat problem

The boundary conditions and geom etry for this problem are set up to simulate an axisymmetric problem on a 3D Cartesian coordinate system. The problem domain is a wedge in the XY plane, going from a knife-edge on axis to finite thickness at the outer part of the cylinder. The large flat faces are reflecting, the outer-cy linder boundary is vacuum, the rightm ost triangular surface is

vacuum, and there is incident ra diation on the leftmost triangular face. In m ore detail, the incoming intensity is specified on the left boundary only along the low-density (blue) m aterial, corresponding to a Planckian intensity at kT=0.3. Everywhere else on this surface, the value of the boundary condition is vacuum. The initial material temperature is kT=0.05 everywhere in the domain, and the simulation is run for 1000 un its of time. A few plots of the simulation results are shown in Figure 18. These plots were generated using PWL as the diffusion solver. As expected, the radiation flows through the thin region and also eventually "eats" its way into the thick region. This is interes ting in itself, but our purpose here is simply to illustrate the performance of CG and GMRES solvers.



Time = 348.523

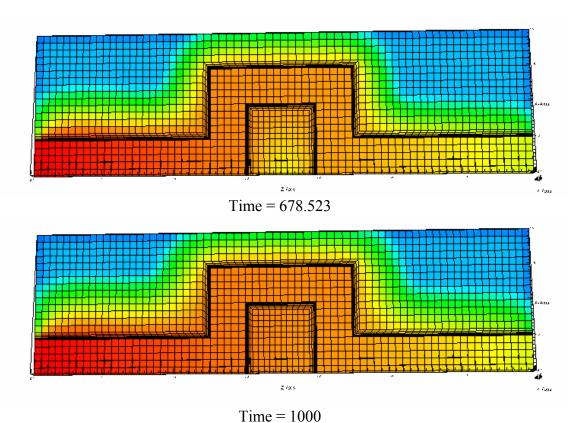


Figure 18: The radiation temperature in the tophat problem shown at different time steps.

We compared the effectiveness of both iterative methods (GMRES for Palmer and PWL, and CG

for PWL) by comparing the number of iterations required to invert the matrix for each reported time step. The preconditioner used for all linear solvers was Algebraic Multigrid.

The results of these calculations, shown in Figure 19, show that CG for PWL requires a factor of three fewer iterations than does GMRES for Palmer's method. (Also, in general GMRES applied to PWL requires slightly fewer iterations than GMRES applied to Palmer's method, which indicates that the PWL matrix is slightly better conditioned than that of Palmer's method.) We further note that in a parallel computing environment, CG has even more advantages over GMRES, because it requires fewer inner products per iteration, and each inner product requires global communication. The combination of reduced storage for the matrix, far fewer iterations, reduced storage of solution-length vectors, and fewer inner products per iteration should make the Galerkin PWL method substantially more efficient than Palmer's method.

Iterations counts (1 processor, tol=1e-8)

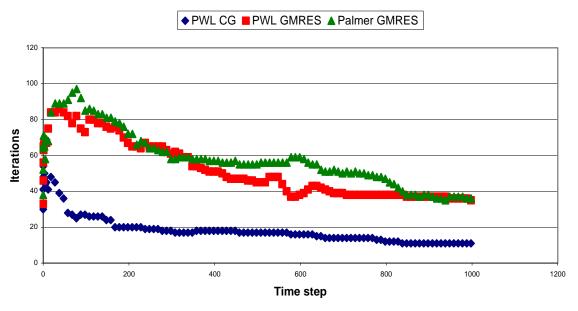


Figure 19: Linear solver comparisons for PWL and Palmer's method for 1 processor.

5. CONCLUSIONS

Our tests show that the Galerkin P WL finite element method applied to the radiation diffusion equation on arbitrary polyhedral meshes has great potential for com putational improvements over previous methods. As we had hoped, the PWL method produces results and behaviors almost identical to those of Palmer's method. Palmer's method has a slight theoretical advantage on orthogonal ("brick") grids in that it generates a highly robus t 7-point discretization whereas PWL generates full 27-point coupling. However, our tests on problems with very high-aspectratio cells did not uncover any poor PWL behavior. Further, the PWL coefficient matrix is SPD with allows for less storage and potentially mo re computationally efficient solutions. We conclude that the Galerkin PWL method is a very attractive option for solving diffusion problems on unstructured grids.

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